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Final Report for Grant Number: F49620-95-1-0210
Managing the Choice of Surrogate Variables and the Use of Approximation Models to Optimize Expensive Functions

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13. ABSTRACT *(Maximum 200 words)*

We propose research in three basic areas. First, it is standard in engineering practice to use approximation models of expensive simulations to drive nonlinear programming algorithms. An open question, which we will investigate using well-established notions from the literature on trust-region methods, is how to manage the interplay between optimization and the fidelity of the approximation models to insure that thc process converges to a reasonable solution of the original design problem. It is also standard in engineering design to reduce the dimension of the optimization problem to be solved by using a technique known as variable linking. We plan to generalize this concept using some recent ideas from the optimization community to design robust ways to decompose a single iteration of any optimization method into a multi-phase process. First, an algorithm is applied to solve subproblems posed on subspaces of lower dimension, and then to solve the full problem on the affine hull defined by the current iterate and the solutions found for the subproblems. Crucial questions remain about the convergence of a practical implementation of this process. Finally, we will continue our research to extend and analyze pattern search methods. Pattern search methods can be successfully applied when only ranking (ordinal) information is available and when derivatives are either unavailable or unreliable. Since these are situations that occur in the design problems of interest, we propose to continue our investigation of pattern search methods. In particular, we will examine robust extensions to handle problems with bound constraints.

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Executive Summary

Major technical advancements have been made on two fronts outlined in our original proposal:

- We developed, analyzed, and implemented a robust software framework, the model management framework (MMF), for using surrogates to optimize computationally expensive nonlinear objective functions. This software implementation has been used to investigate the effectiveness of the MMF approach when applied first to several academic test problems and then to a realistic engineering design problem from Boeing. This conforms with our stated goal in the proposal that we would work closely with Boeing to make sure that our software applies to real problems. The implementation (in Fortran 90) is publicly available and has been transferred to our collaborators at Boeing where it will be developed to investigate such problems as the design of helicopter rotor blades, jet engine nozzles, and wings.

- We developed extensions to and analysis for pattern search methods for nonlinear optimization. We have been able to develop variants to handle both bound and general linear constraints, as well as to develop a rigorous understanding of the minimal amount of information that must be generated at a single iteration to ensure progress of the optimization process. The analysis for bound constraints, as well as the understanding of the minimal amount of information that must be generated a single iteration, form the basis for the convergence analysis of the MMF. The extensions for general linear constraints, which also allows for a more frugal implementation for bound constraints, is expected to be incorporated into our MMF software framework in the near future.

Outcomes on both these fronts exceeded the expectations outlined in our original proposal and resulted in multiple papers, several reports, and a dissertation.

In addition to the two main objectives outlined above, the grant was also used to support the development of multiobjective optimization tools. The development of these tools forms the basis of the dissertation of Indraneel Das. Boeing is beginning to apply these tools to some of their design problems. So far, no details are available, but we have been promised some success stories to pass on to AFOSR and DOE, the sources of graduate student support for Dr. Das, who is now with IBM.

Personnel Supported:

Faculty: J. E. Dennis
Virginia Torczon
M. W. Trosset

Postdoctoral Researcher: Douglas Moore

Graduate Students: Indraneel Das (Thesis: "Nonlinear Multicriteria Optimization and Robust Optimality")
David Serafini (Thesis: "A Framework for Managing Models in Nonlinear Optimization of Computationally Expensive Functions")

Publications:

Published:

- (Natalia Alexandrov, J. E. Dennis, Jr., Robert Michael Lewis, and Virginia Torczon) "A Trust Region Framework for Managing the Use of Approximation Models in Optimization". *Structural Optimization*, 15(1), pp 16–23, 1998.

- (D. M. Cox, K. A. Bayles, and M. W. Trosset) "Category and Attribute Knowledge Deterioration in Alzheimer's Disease". *Brain and Language*, 52, pp 536–550, 1996.

- (Indraneel Das and J. E. Dennis) "A Closer Look at Drawbacks of Minimizing Weighted Sums of Objectives for Pareto Set Generation in Multicriteria Optimization Problems". *Structural Optimization*, 14(1), pp. 63–69, 1997.

- (J. E. Dennis and Natalia Alexandrov) "Multilevel Algorithms for Nonlinear Optimization", in *Optimal Design and Control*, edited by J. Borggaard, J. Burkardt, M. Gunzburger, and J. Peterson, Birkhäuser PSCT 19, pp. 1-22, 1995.

- (J. E. Dennis, M. El-Alem, M. C. Maciel) "A Global Convergence Theory for Trust-Region-Based Algorithms for Equality Constrained Optimization". *SIAM Journal on Optimization*, 7(1), pp. 177–207, 1997.

- (J. E. Dennis and Virginia Torczon) "Managing Approximation Models in Optimization", in *Multidisciplinary Design Optimization: State-of-the-Art*, edited by Natalia M. Alexandrov and M. Y. Hussaini, SIAM, 1997, pp. 330–347.

- (J. E. Dennis and Luís N. Vicente) "On the Convergence Theory of Trust-Region-Based Algorithms for Equality-Constrained Optimization". *SIAM Journal on Optimization*, 7(4), pp. 927–950, 1997.

- (J. E. Dennis and Luís N. Vicente) "Trust-Region Interior-Point Algorithms for Minimization Problems with Simple Bounds", in *Applied Mathematics and Parallel Computing: Festschrift für Professor Dr. Klaus Ritter*, edited by H. Fischer, B. Riedmüller, and S. Schaffler, Springer, Heidelberg, pp. 97-109, 1996.

- (A. J. Kearsley, R. A. Tapia, and M. W. Trosset) "An Approach to Parallelizing Isotonic Regression", in *Applied Mathematics and Parallel Computing: Festschrift für Professor Dr. Klaus Ritter*, edited by H. Fischer, B. Riedmüller, and S. Schaffler, Springer, Heidelberg, 1996.

- (C. K. Tomoeda, K. A. Bayles, M. W. Trosset, T. Azuma, A. McGeagh) "Cross-sectional Analysis of Alzheimer Disease Effects on Oral Discourse in a Picture Description Task", *Alzheimer Disease and Associated Disorders*, 10(4), pp. 204–215, 1996.

- (Virginia Torczon) "On the Convergence of Pattern Search Methods", *SIAM Journal on Optimization*, 7(1), pp. 1–25, 1997.

- (M. W. Trosset) Book Review: *Biplots. Technometrics*, 39(3), pp 339–340, 1997.

- (M. W. Trosset) "Numerical Algorithms for Multidimensional Scaling", in *Classification and Knowledge Organization*, edited by R. Klar and O. Opitz, Springer, Heidelberg, 1997, pp. 80–92.

- (M. W. Trosset and A. W. Kaszniak) "Measures of Deficit Unawareness for Predicted Performance Experiments". *Journal of the International Neuropsychological Society*, 2(4), pp. 315–322, 1996.

- (M. W. Trosset and B. N. Sands) "On the Choice of a Discrepancy Functional for Model Selection". *Communications in Statistics—Theory and Methods*, 24(11), pp 2841–2863, 1995.

Accepted for Publication:

- (Andrew J. Booker, J. E. Dennis, Jr., Paul D. Frank, David B. Serafini, Virginia Torczon, and Michael W. Trosset) "A Rigorous Framework for Optimization of Expensive Functions by Surrogates". Accepted, subject to suitable revision, for publication in *Structural Optimization*.

- (Andrew J. Booker, J. E. Dennis, Jr., Paul D. Frank, David B. Serafini, and Virginia Torczon. "Optimization Using Surrogate Objectives on a Helicopter Test Example". To appear in *Optimal Design and Control*, edited by J. Borggaard, J. Burns, E. Cliff, and S. Schreck, Birkhauser.

- (Indraneel Das and J. E. Dennis) "Normal-Boundary Intersection: A New Method for Generating Pareto Optimal Points in Nonlinear Multicriteria Optimization Problems". To appear in *SIAM Journal on Optimization*.

3

- (J. E. Dennis, Matthias Heinkenschloss, Luis Vicente) "Trust-Region Interior-Point Algorithms for a Class of Nonlinear Programming Problems". To appear in *SIAM Journal on Control and Optimization.*

- (A. J. Kearsley, R. A. Tapia, and M. W. Trosset) "The Solution of the Metric STRESS and SSTRESS Problems in Multidimensional Scaling by Newton's Method". To appear in *Computational Statistics.*

- (Robert Michael Lewis and Virginia Torczon) "Pattern Search Methods for Bound Constrained Minimization". To appear in *SIAM Journal on Optimization.*

- (M. W. Trosset) Comment on "Consulting: Real Problems, Real Interactions, Real Outcomes". To appear in *Statistical Science*, 13(1), 1999.

- (M. W. Trosset) "Distance Matrix Completion by Numerical Optimization". To appear in *Computational Optimization and Applications.*

- (M. W. Trosset) "A New Formulation of the Nonmetric STRAIN Problem in Multidimensional Scaling". To appear in *Journal of Classification.*

- (M. W. Trosset and R. Mathar) "On the Existence of Nonglobal Minimizers of the STRESS Criterion for Metric Multidimensional Scaling". To appear in *American Statistical Association 1997 Proceedings of the Statistical Computing Section.*

- (M. W. Trosset and G. N. Phillips) "Deriving Interatomic Distance Bounds from Chemical Structure". To appear in the proceedings of the 1997 Joint Summer Research Conference in the Mathematical Sciences on Statistics in Molecular Biology.

Submitted for Publication:

- (Natalia Alexandrov and J. E. Dennis) "A Class of General Trust-Region Multilevel Algorithms for Systems of Nonlinear Equations and Equality Constrained Optimization: Global Convergence Theory". Submitted for publication.

- (J. E. Dennis, M. El-Alem and Karen Williamson) "A Trust-Region Algorithm for Least-Squares Solutions of Nonlinear Systems of Equalities and Inequalities". Submitted for publication.

- (J. E. Dennis and Robert Michael Lewis) "A Comparison of Nonlinear Programming Approaches to an Elliptic Inverse Problem and a New Domain Decomposition Approach". Submitted for publication.

- (Robert Michael Lewis and Virginia Torczon) "Pattern Search Algorithms for Linearly Constrained Minimization". submitted to *SIAM Journal on Optimization.*

- (Robert Michael Lewis and Virginia Torczon) "Rank Ordering and Positive Bases in Pattern Search Algorithms". In revision for *Mathematical Programming.*

- (M. W. Trosset and Virginia Torczon) "Numerical Optimization Using Computer Experiments". In revision for *Technometrics*.

- (M. W. Trosset) "Computing Distances Between Convex Sets and Subsets of the Positive Semidefinite Matrices". Submitted to *SIAM Journal on Optimization*.

- (M. W. Trosset) "Distance Matrix Completion by Numerical Optimization". Submitted to *Computational Optimization and Applications*.

- (M. W. Trosset) "The Formulation and Solution of Multidimensional Scaling Problems", In revision for *Statistical Science*.

- (M. W. Trosset, K. Baggerly and K. Pearl) "Another Look at the Additive Constant Problem in Multidimensional Scaling". Submitted to *Psychometrika*.

Interactions and Transitions:

Public Presentations:

J. E. Dennis

- "Managing Model Approximations in Multidisciplinary Optimization". University of Florida; February 9, 1996; Gainesville, Florida.

- "Managing Model Approximations in Multidisciplinary Optimization". Fifth SIAM Conference on Optimization; May 23, 1996; Victoria, British Columbia, Canada.

- Short Course: "Trust Region Algorithms for Nonlinear Programming". IFORS Annual Meeting; July 11, 1996; Vancouver.

- "The Boeing/IBM/Rice Collaboration for Multidisciplinary Optimization". Boeing Helicopters; July 30, 1996; Philadelphia.

- "Unifying Concepts for The Boeing/IBM/Rice Collaboration for Multidisciplinary Optimization". Boeing Research & Technology; August 8, 1996; Bellevue, Washington.

- "Trust Region Interior Point Algorithms for Computational Engineering; The TRICE Software". August 21, 1996, Boeing Research & Technology, Bellevue, Washington.

- "Managing Model Approximations in Multidisciplinary Optimization". AIAA-MDO Symposium; September 5, 1996; Bellevue, Washington.

- "Managing Model Approximations in Multidisciplinary Optimization". NWNAS; September 21, 1996; Vancouver.

- "Managing Model Approximations in Multidisciplinary Optimization". INFORMS Annual Meeting; November 4, 1996; Atlanta.

- "Managing Model Approximations in Multidisciplinary Optimization". Mathematics Research Institute; January 6, 1997; Oberwolfach, Germany.

- "Managing Model Approximations in Multidisciplinary Optimization". Boeing Research and Technology; March 26, 1997; Seattle.

- Plenary Talk: "Managing Model Approximations in Multidisciplinary Optimization". SIAM SEAS Meeting; April 4, 1997; Raleigh.

- "Managing Model Approximations in Multidisciplinary Optimization". University of Washington; April 8, 1997; Seattle.

- "Managing Model Approximations in Multidisciplinary Optimization". Rice CAAM Departmental Seminar; April 21, 1997; Houston.

- Plenary Talk: "Trust Region Interior Point Algorithms for Computational Engineering; The TRICE Software". Montreal Optimization Days; May 5, 1997; Montreal.

- "Managing Model Approximations in Multidisciplinary Optimization"; Washington State University; May 14, 1997; Pullman.

- Plenary Talk: "Trust Region Interior Point Algorithms for Computational Engineering; The TRICE Software". Constructive Mathematics Meeting; Simon Fraser University; June 23, 1997; Vancouver.

- "The Rice Accomplishments under the NASA/IBM CRA". NASA Ames Research Center; June 30, 1997; Mountain View.

- "Managing Model Approximations in Multidisciplinary Optimization". University of Trier; August 21, 1997; Trier, Germany.

- "Managing Model Approximations in Multidisciplinary Optimization". International Mathematical Programming Symposium; August 25, 1997; Lausanne.

- Presidential Address: "Optimization: An Essential Tool for Decision Support". International Mathematical Programming Symposium; August 25, 1997; Lausanne.

- "A Sabbatical in Industry". Rice Engineering Alumni; September 17, 1997; Houston.

- "Surrogate Optimization of Expensive Functions". American Mathematics Society Regional Meeting; November 9, 1997; Albuquerque, NM.

- "Surrogate Optimization of Expensive Functions". Computer Science Affiliates Meeting, Rice University; November 10, 1997; Houston.

- "Surrogate Optimization of Expensive Functions". Sandia Laboratory; November 11, 1997; Albuquerque, NM.

- "Career Opportunities for Applied Mathematicians". Mathematics Club, St. Johns School; November 30, 1997; Houston.

- "Surrogate Optimization of Expensive Functions". Argonne National Laboratory; December 15, 1997; Argonne.

- "Surrogate Optimization of Expensive Functions". WPI Math Department; January 23 1998; Worcester.

- "Surrogate Optimization of Expensive Functions". IBM T. J. Watson Research Center; January 26 1998; Yorktown Heights.

- "Surrogate Optimization of Expensive Functions". IBM CITI Site Visit, Rice University; February 25, 1998; Houston.

- "Surrogate Optimization of Expensive Functions". Department of Mathematics & Statistics, University of Canterbury; March 19, 1998; Christchurch, NZ.

- "Trust Region Interior Point Algorithms for Engineering Design". Department of Mathematics & Statistics, University of Canterbury; March 19, 1998; Christchurch, NZ.

- "Optimization, An Essential Tool for Decision Support". Dean's Distinguished Lecture, University of Canterbury; April 7, 1998; Christchurch, NZ.

- "Surrogate Optimization of Expensive Functions". Statoil Site Visit, CITI, Rice University; April 29, 1998; Houston.

- "Rice Contributions to Research in Optimization, Automatic Differentiation, and Interior Point Methods". Distinguished Faculty Lecture, 30th Anniversary of the Rice Computational and Applied Mathematics Department; May 16, 1998; Houston.

Douglas Moore:

- "Designing an Object Oriented Optimization System". Fifth SIAM Conference on Optimization; May 23, 1996; Victoria, British Columbia, Canada.

- "Copilot — Successive Linear Programming with Trust Regions for Constrained Optimization". International Mathematical Programming Symposium; August 27, 1997; Lausanne.

David Serafini:

- "Software for Managing Model Approximations in Multidisciplinary Optimization". Fifth SIAM Conference on Optimization; May 23, 1996; Victoria, British Columbia, Canada.

- "Software for Managing Model Approximations in Multidisciplinary Optimization". Computational Aerosciences Workshop, NASA Ames Lab; August 15, 1996; Sunnyvale, California.

- "Progress at Rice on SP2 use in MDO". IBM Workshop, NASA Ames Lab; August 16, 1996; Sunnyvale, California.

- "Software for Managing Model Approximations in Multidisciplinary Optimization". AIAA-MDO Symposium; September 5, 1996; Bellevue, Washington.

Virginia Torczon:

- Colloquium talk: "Pattern Search Methods: Theory and Practice". Department of Computer Science, College of William & Mary; March 17, 1995; Williamsburg, Virginia.

- Invited talk: "A Specific Algorithm for Managing Approximation Models in Optimization". CRPC Research Symposium and Annual Meeting, Rice University; March 23, 1995; Houston, Texas.

- Colloquium talk: "Pattern Search Methods for Nonlinear Optimization". Department of Computer and Mathematical Sciences, University of Houston—Downtown; March 29, 1995, Houston, Texas.

- Colloquium talk: "Pattern Search Methods: Theory and Practice". Department of Computational and Applied Mathematics, Rice University; April 17, 1995; Houston, Texas.

- Invited article: "Pattern search methods for nonlinear optimization". SIAG/OPT Views-and-News: A Forum for the SIAM Activity Group on Optimization, No. 6; Spring, 1995.

- Colloquium talk: "Pattern Search Methods for Nonlinear Optimization on Parallel Machines". Department of Computer Science, Old Dominion University; September 27, 1995; Norfolk, Virginia.

- Colloquium talk: "Pattern Search Methods for Nonlinear Optimization on Parallel Machines". Operations Research Interest Group, College of William and Mary; November 14, 1995; Williamsburg, Virginia.

- Colloquium talk: "Pattern Search Methods for Nonlinear Optimization on Parallel Machines". Department of Computer Science, Virginia Polytechnic Institute and State University; March 6, 1996; Blacksburg, Virginia.

- Invited talk: "Managing Approximation Models in Optimization". INFORMS Conference on Information Systems & Technology; May 7, 1996; Washington, D.C.

- Plenary talk: "Direct Search Methods". Fifth SIAM Conference on Optimization; May 21, 1996; Victoria, British Columbia, Canada.

- Plenary talk: "Managing Approximation Models in Optimization". ICASE Workshop on Approximation; August 14, 1996; NASA Langley Research Center, Hampton, Virginia.

- Invited talk: "A Pattern Search Approach to Managing Approximation Models in Engineering Optimization". INFORMS Atlanta Fall 1996; November 4, 1996; Atlanta.

- Contributed talk: "From Evolutionary Operation to Parallel Direct Search: Pattern Search Algorithms for Numerical Optimization". Interface '97; May 16, 1997; Houston.

- Invited short Course: "A Parallel Optimization Primer" (with Robert Michael Lewis). CRPC Annual Research Meeting; May 20, 1997; Houston.

- Invited short course: "A Parallel Optimization Primer" (with Robert Michael Lewis). Aeronautical Systems Center, Wright–Patterson Air Force Base; May 29, 1997; Dayton, Ohio.

- Contributed talk: "Pattern Search Methods for Engineering Optimization". Electronic Prototyping, Air Force Office of Scientific Research; May 29, 1997; Blacksburg, Virginia.

- Invited talk: "Rank Ordering and Positive Bases in Pattern Search Methods". SIAM Annual Meeting; July 17, 1997; Palo Alto, California.

- Contributed talk: "Robust Derivative-Free Methods for Linearly Constrained Minimization". International Symposium on Mathematical Programming; August 26, 1997; Lausanne.

M. W. Trosset:

- "Some Fundamental Ideas in Stochastic Optimization". Departments of Statistics and Computational & Applied Mathematics, Rice University; November 27, 1995; Houston.

- "General Issues in the Optimization of Expensive Functions". Boeing/IBM/Rice Workshop on Approximation Models, Rice University; February 22, 1996; Houston.

- Plenary Lecture: "Numerical Algorithms for Multidimensional Scaling". 20th Annual Conference of Gesellschaft für Klassifikation e.V.; March 7, 1996; Freiburg, Germany.

- "Computational Methods for Stochastic Minimum Distance Estimation". Department of Operations Research, Naval Postgraduate School; April 8, 1996; Monterey, California.

- "Computational Methods for Stochastic Minimum Distance Estimation". Department of Systems & Industrial Engineering, University of Arizona; May 2, 1996; Tucson, Arizona.

- "Local Quadratic Models in Stochastic Optimization" (Minisymposium on Beyond Taylor Series Approximations: The Use of Alternative Models in Nonlinear Programming". Fifth SIAM Conference on Optimization; May 23, 1996; Victoria, British Columbia, Canada.

- Short Course: "Optimization Problems in Multidimensional Scaling. Workshop on Classification and Optimization in Statistics". Rice Institute for Mathematical Sciences, Rice University; July 15–19, 1996; Houston.

- "General Issues in the Optimization of Expensive Functions". Workshop on Approximation Models, Institute for Computer Applications in Science & Engineering; August 15, 1996; Langley, Virginia.

- "Data Box Algorithms for Molecular Conformation". Fall Symposium 5: Computational Biology—Methods in Biomolecular Imaging, American Society for Biochemistry & Molecular Biology; October 25–28, 1996; Whistler, British Columbia, Canada.

- "On the Fundamental Role of Interior-Point Methodology in Constrained Optimization". Fall Symposium 5: Computational Biology—Methods in Biomolecular Imaging, American Society for Biochemistry & Molecular Biology; October 25–28, 1996; Whistler, British Columbia, Canada.

- "New Extensions of Classical Multidimensional Scaling". Department of Biostatistics, University of Colorado Health Science Center; November 14, 1996; Denver.

- "New Extensions of Classical Multidimensional Scaling". Department of Mathematics, University of Colorado at Denver; November 18, 1996; Denver.

- "New Extensions of Classical Multidimensional Scaling". Department of Statistics, Virginia Polytechnic Institute & State University; December 5, 1996; Blacksburg, Virginia.

- "Inferring Molecular Conformation from Interatomic Distances". W.M. Keck Center for Computational Biology, Rice University; February 21, 1997; Houston.

- "Numerical Optimization Using Computer Experiments". Department of Statistics, Rice University; April 21, 1997; Houston.

- "Applications of Multidimensional Scaling to Molecular Conformation". Interface '97; May 15–17, 1997; Houston.

- "Inferring Molecular Structure from Interatomic Distances". Statistics in Molecular Biology, Joint Summer Research Conference in the Mathematical Sciences; June 22–26, 1997; Seattle.

- Short Course: "Introduction to Dimension Reduction". Workshop on Statistical Function Estimation, Image Understanding and Optimization; Rice Institute for Mathematical Sciences, Rice University; June 2–13, 1997; Houston.

- "Approximation and Modelling in Stochastic Optimization". Workshop on Approximations and Surrogates, Institute for Computer Applications in Science & Engineering; July 21–23, 1997; Langley, Virginia.

- "On the Existence of Nonglobal Minimizers of the STRESS Criterion for Metric Multidimensional Scaling". Joint Statistical Meetings; August 10–14, 1997; Anaheim, California.

Consultative and Advisory Functions:

J. E. Dennis

- Organized a visit to Rice University on March 20, 1996 at the request of four young scientists from Lever Brothers for the purpose of their becoming acquainted with new technologies.

- Arranged for Jennifer Rich, one of his Engineering Optimization students, to do a class project at Texaco on optimal blending of unleaded gasoline; April, 1996.

- Met with Dr. Francisco Brana of Shell Development several times to discuss MDO approaches to chemical process control; 1996.

- Chaired of the External Review in Computer Science, Duke University; Spring, 1996.

- Interdisciplinary Mathematics Ph.D. Program Advisory Committee, University of Puerto Rico; October, 1996.

- Applied Mathematics Center Advisory Committee, University of Florida; November, 1996.

- NSF Renewal Site Visit Team to IMA, University of Minnesota; February 1997.

- University of Chicago Computer Science Review Committee; December 15-17, 1997.

- One of 4 Academics on DOE Panel to define DOE2000 Program, Lawrence Berkeley Labs; Feb 9-10, 1998.

- Organized Boeing/IBM/Rice collaboration workshop in Houston, (with Teresa Parks); Feb 19-20, 1998.

Virginia Torczon

- Consultant in Residence, ICASE, NASA Langley Research Center, Hampton, Virginia, October, 1995–present.

- Invited Participant: 1997 Petaflops Algorithms Workshop (PAL '97) (jointly sponsored by DARPA, DOE, NASA, NSA, and NSF); April 13–18, 1997; Williamsburg, Virginia.

- Served on two National Science Foundation Scientific Computing Research Environments for the Mathematical Sciences (SCREMS) panels, April, 1996 and February 1997.

Douglas Moore

- Consulted with Juan Meza of Sandia National Laboratories (CA) on issues of numerical software design.

Transitions:

Earthquake Simulation

In 1996, Rice Professors Steve Cox and Joel Conte used PDS to solve for the first time an optimization formulation of the problem of retrofitting existing buildings to suppress earthquake vibrations. Conte also used PDS to solve an inverse problem to determine earthquake source location.

Sandia Labs OPT++ Engineering Optimization System

In 1996, the constraints version of PDS(MDS) was incorporated into the Sandia Labs OPT++ Engineering Optimization System of Dr. Juan Meza (510)294-2425 with the help of David Serafini and Doug Moore. Moore collaborated with Meza in redesigning the object oriented OPT++ system.

Sandia Chemical Vapor Deposition Problem

The TRICE modules for optimization with simulation constraints were used to solve a chemical vapor deposition problem in silicon wafer production. This code performed better than another interior point NLP code based on different principles.

Boeing Parts Nesting System

PDS continues to be used in the Boeing Parts Nesting System for Just-in-Time manufacturing of aircraft parts.

PDS Software

The latest version of the PDS (Parallel Direct Search) software for unconstrained optimization problems will be installed in the Network-Enabled Optimization System (NEOS), managed by the Mathematics and Computer Science Division, Argonne National Laboratory, Illinois, at the invitation of Jorge Moré.

Torczon has been invited to submit PDS for inclusion in the National HPCC Software Exchange (NHSE), a program to actively promote software sharing and reuse within and across the participating agencies (NIST, AHCPR, DARPA, NOAA, NASA, EPA, VA, NIH, NSF, ED, NSA, and DOE) in the federal High Performance Computing and Communications (HPCC) Program. (http://www.nhse.org)

Torczon has also been invited to place PDS in PINEAPL, a European project to develop parallel numerical library software for industrial applications, managed by the Numerical Algorithms Group (NAG) Ltd., United Kingdom. (http://extweb.nag.co.uk/projects/PINEAPL.html).

In addition to including the parallel variant of PDS in PINEAPL, NAG has expressed an interest in incorporating the sequential variant into their commercial numerical software libraries. (http://www.nag.co.uk/numeric.html)

Nozzle Design

Our group is working with a group in Boeing Commercial Airplane Group (BCAG) to reduce the cycle time for designing nozzles. A nozzle is the inside part of the engine housing, and its design is affected by the design of the more "upstream" components. This means that many of the design changes involving other airplane components force a redesign of the nozzle as well.

A nozzle design is specified by 100 parameters, 90 of which are fixed by other considerations. The system is governed by a 2D Navier Stokes coupled with NASTRAN, a commercial structures code. It takes about 3 hours on an SGI Challenge to get one function value. The current length of a design cycle is two weeks. We expect to reduce that to approximately one day.

Contact: Greg Shubin (425) 865-3516.

Planform Design

Our group is working with another BCAG group that does planform design. Here, they are hoping for better planforms, not just reduced cycle time. The planform is the shape of the wing as viewed from above. It is a tricky design problem that involves a couple of dozen variables and some interesting constraints. For example, the fuel is outboard on the wings, and the wings must be swept back for performance. One constraint is that the plane must not fall over backwards when the tanks are filled while the plane is on the ground. This problem involves multiple objectives.

Contact: Greg Shubin (425) 865-3516.

High-Speed Cutting Tool Design

High-speed machine tools encounter the metal at over 300 mph. At that speed, the metals are not fully solid. This allows more complicated parts to be machined in a single piece. Many large airplane parts are currently assembled from components that were machined separately. If, during airplane assembly, one of these parts doesn't quite fit, work stops and a supervisor is called in to approve the use of shims to make it fit. The Boeing plant in Wichita found a significant reduction in the need for this "shimming" when large parts were machined as a single piece using a high-speed machine tool.

Since this is a new technique, no one yet knows how to design a really good cutting tool. This is a three-variable, very expensive multiobjective problem.

Contact: Greg Shubin (425) 865-3516.

Helicopter Rotor Blade Design

This is the problem we have been working on for the longest time. Wake simulation is the hard part of the problem, and the effects at the tip of the rotor blade are the most difficult to

simulate. It takes about 4 hours on 16 fat nodes of an SP2. Our group at Boeing managed to build a response surface model for the spline coefficients of the output of the full potential rotor discipline as a function of the spline coefficients of the input to that code, which is the output from the coupled simulation involving thermal analysis, structural analysis, and aerodynamics analysis. This new model reduces the cost to minutes and the bandwidth of the coupling from 100s to 10s. We will be experimenting with the 14 objective functions they want to trade off using this cheaper code.

Contact: Greg Shubin (425) 865-3516.

Model Management Framework Software

The framework software has been transferred to our collaborators at Boeing. They will use the framework to develop model management algorithms that are specialized for their applications and capabilities.

Contact: Greg Shubin (425) 865-3516.

SLP Software

COPILOT has been used to solve a problem in multidisciplinary optimization from NASA Langley, as well as on standard benchmark sets. The software will appear shortly on the NEOS server, and will be made available over the Internet.

Contact: Natalia Alexandrov (757) 864-7059

Inventions, or Patent Disclosures:

None.

Honors/Awards:

J. E. Dennis

- President of the Mathematical Programming Society.

- Member, International Program Committee of the Mathematical Programming Society (1987—).

- Founding Editor-In-Chief of *SIAM Journal on Optimization.*

- Served on and chaired numerous panels and visiting committees.

- Advisory Editor, *Mathematics of Operations Research,* (1992—).

- Served two terms on the SIAM Council.

- Fulbright Lecturer to Argentina.

Virginia Torczon

- Invited to join the editorial board of the new SIAM Book Series in Advances in Design and Control, John A. Burns, Editor-in-Chief.

- Elected Program Director, SIAM Activity Group on Optimization, January 1, 1998– December 31, 2000.

- Invited to organize the Cluster on Nonlinear Programming for INFORMS Seattle, October 25–28, 1998.

- Invited to serve as Member, Organizing Committee, Sixth SIAM Conference on Optimization; Atlanta, Georgia; May 10–12, 1999.

- Elected to SIAM Council, Society for Industrial and Applied Mathematics; January 1, 1997–December 31, 1999.

- Appointed to SIAM Committee on Committees and Appointments; January 1, 1997– December 31, 1998.

- Co-chair, Eighth SIAM Conference on Parallel Processing for Scientific Computing; Minneapolis, Minnesota; March 14–17, 1997.

- Appointed to the Technical Steering Committee, Optimization and Automatic Differentiation, Center for Research in Parallel Computation; effective November 1996.

- Gave plenary address *Direct Search Methods* at 5th SIAM Conference on Optimization, May 1996.

- Member, Tutorial Committee, Supercomputing '95, November 1995.

- Secretary, SIAM Activity Group on Supercomputing, January 1, 1994–December 31, 1996.

15

Final Report for Grant Number: F49620-95-1-0210
Managing the Choice of Surrogate Variables and the Use of
Approximation Models to Optimize Expensive Functions

The Context of the Research

Mathematically, the problem we solve can be expressed as:

$$\text{minimize} \quad f(x) \tag{1}$$
$$\text{subject to} \quad x \in \mathcal{B} \equiv \{x \mid a \leq x \leq b\},$$

where $f : \Re^n \to \Re \cup \{\infty\}$, $a, b \in \Re^n$, and $a \leq b$ means that each coordinate satisfies $a_i \leq b_i$.

Problem (1) is an optimization problem with simple bound constraints. Most problems also include other types of constraints. Our helicopter examples include an additional linear inequality constraint. Usually, such constraints are managed either by using them to eliminate one of the variables or simply by assigning a large function value to infeasible points, although the latter approach can fail in theory. Recent analysis for pattern search methods [32] eliminates this shortcoming and can be extended to our model management framework. Managing nonlinear constraints, especially equality constraints, is an issue that we have not yet addressed in the model management framework.

Some key properties of our target problems are:

1. The number of decision variables x is reasonably small, say $n \leq 100$.

2. It is impractical to accurately approximate derivatives of f.

3. The routines that evaluate $f(x)$ may fail for some feasible x at the same cost as if a value had been obtained.

4. If x violates any of the bound constraints, then $f(x)$ may not be available.

5. The computation of $f(x)$ is very expensive and the values obtained may have few correct digits.

Although the number of *optimization* variables is reasonably small, the *total* number of variables in the problem usually is large. Typically, $f(x)$ is expensive to evaluate because there are large numbers of ancillary or system variables that must be determined for each choice of x before $f(x)$ can be evaluated. For the helicopter rotor blade problem, x specifies a coupled set of partial differential equations (PDEs) that must be solved in order to obtain dependent system variables that are then used to evaluate $f(x)$. The coupling of PDEs via some iterative method, most often the notoriously unreliable successive substitution approach, explains the third of our assumptions, since the method may run for many iterations and not converge.

The second and third of our intrinsic assumptions make quasi-Newton methods difficult to apply. Choosing a finite-difference step size to approximate derivatives is a difficult and crucial part of getting a finite-difference quasi-Newton method to work. This difficulty is compounded by the fact that we may not be able to compute the function value at the step

size selected. We hope that as automatic differentiation technology advances, actual derivatives can be used rather than finite-difference approximations. However, the last assumption is again relevant because quasi-Newton methods are affected by function inaccuracies [23].

If we discount the expense of evaluating $f(x)$, then direct search methods [51, 54, 53] avoid many of the difficulties that we have identified. Indeed, parallel direct search (PDS) [21, 50] solved 10, 31, and 56 variable instances of the helicopter rotor blade design problem. Direct search methods are sampling methods and so typically many function values are required to solve the problem. Furthermore, the "curse of dimensionality" also plays a major role; problems in higher dimensions require significantly more function evaluations than do problems in lower dimensions. The curse of dimensionality can be ameliorated somewhat by exploiting the fact that PDS is "embarrassingly" parallel and can be installed easily on any parallel or distributed computing platform that supports the message-passing interface (MPI).

The unifying theme of this project has been that we wished to apply a generalized pattern search method *indirectly* using surrogates as guides to make adaptive choices as to where to evaluate the objective function. Our motivation was that surrogates, which are chosen to be inexpensive to evaluate, could be used to avoid as much as possible unnecessary computation of the expensive objectives. A major goal of our research has been to combat the curse of dimensionality, which often hinders the effectiveness of pattern search methods when applied to problems in higher dimensions. However, we maintain the structure of pattern search methods to ensure our method is robust.

In fact, our goal was realized. Boeing is currently most interested in the 31-variable helicopter problem—PDS and MMF greatly reduced the baseline objective function value provided by our collaborators at Boeing. While PDS successfully solved this problem, the MMF solved it with fewer evaluations of the objective (5465 and 237, respectively). In addition, we have made useful extensions to the pattern search methods and their convergence theory—extensions which support both the implementation and analysis of the MMF.

Summary of Results

In the proposal "Managing the Choice of Surrogate Variables and the Use of Approximation Models to Optimize Expensive Functions," we proposed research in three basic areas:

1. The use of approximation models as surrogates for expensive functions in optimization;

2. Extensions of pattern search methods to handle optimization problems with bound constraints; and

3. The use of subspace/surrogate variable techniques in optimization.

We made dramatic progress on the first two topics, including some findings that had not been anticipated by our original proposal.

The third topic is still important, but, frankly, both our model management framework software (MMF) and our parallel direct search software (PDS) performed much better and for much larger problems than we had ever anticipated. Thus progress in the first two areas

took precedence. However, the time will come when new approaches will be needed to tackle even larger problems, and we still believe that our subspace approach is promising.

In this report we summarize accomplishments pertaining to these topics. More details can be found in the references [1, 7, 8, 9, 10, 22, 30, 31, 32, 41, 52, 55].

Optimization using Surrogate Objectives

This was the major thrust of F49620-95-1-0210. Our proposals were based on the model management framework proposed by Dennis and Torczon [22], in which techniques that do not rely on explicit approximations to gradients of the objective function were employed. We were able to develop a simpler and more direct version of model management, which is implemented in the MMF software.

The results of our research on this topic are summarized in the dissertation of David Serafini and in our papers [9] and [10]; they include a through discussion and analysis of our simpler model management strategy. The remainder of Serafini's dissertation is devoted to developing a software prototype that is sufficiently flexible to accommodate both a variety of algorithms for the optimization and, importantly, a variety of classes of objective function approximations. The resulting paper [10] is undergoing final revision now.

The MMF software has produced consistently excellent results with approximations chosen to be either variable-order multivariate polynomial interpolants to the objective function [20] or interpolants from the design and analysis of computer experiments (DACE) literature, which are in wide use at Boeing [5, 6]. The DACE approximations are so-called kriging models which originated in the geophysics community but have gained wide currency in the statistical community (see [4, 5, 11, 12, 13, 16, 17, 26, 27, 29, 36, 38, 39, 40, 42, 45, 47, 56, 57, 58]). Trosset and Torczon [55] have preliminary numerical results to suggest that even a greatly simplified kriging approximation can be more efficient for optimization with scarce resources than the one-shot experiment approach often suggested in the computer experiment literature.

Alexandrov, Dennis, Lewis and Torczon [1] proposed an analogous management strategy for first-order methods (methods that do explicitly approximate gradients) and extended the convergence theory for trust-region methods to establish global convergence to a local solution. The importance of this work is that it shows how much simpler a model management strategy can be, even for the constrained case, if the surrogates are assumed to match the derivatives of the true objective and constraint functions.

Pattern search methods

Our analysis of the MMF has been based on the definition and convergence analysis of pattern search methods, for which a brief, general, less technical introduction can be found in [53].

Torczon [52] identified a common structure underlying what had been regarded as a disparate collection of search techniques based on practical heuristics. This structure defines the class of pattern search methods, for which Torczon [52] also established a global convergence theory in the case of unconstrained optimization. Besides providing a rigorous foundation

for the folklore that pattern search methods are robust in practice, the convergence analysis is theoretically interesting because of its close relationship to the extant analysis for quasi-Newton methods (see [35]).

Recent research papers by Lewis and Torczon [30, 31, 32] build on Torczon [52] . Lewis and Torczon extended the convergence analysis to the case of bound-constrained [30] optimization problems. An interesting algorithmic consequence of this work is that it possible, with only simple modifications to the original methods, to construct pattern search methods that are guaranteed to converge to a Karush-Kuhn-Tucker point.

Lewis and Torczon [32] further extends the theory to the case of general linear constraints. The algorithmic consequences of this analysis are more provocative as no existing pattern search method satisfies the conditions necessary to guarantee convergence to a Karush-Kuhn-Tucker point, nor can one be obtained from simple modifications of the original methods. They were encouraged by the discovery that a similar line of analysis by May [33] led to promising numerical results when implemented and tested.

Lewis and Torczon [31] also generalized the convergence analysis found in Torczon [52]; the effect of this generalization was to (almost) halve the worst case cost of a single iteration of a pattern search method in the unconstrained case by reducing the maximum number of function evaluations required from $2n$ to $n + 1$. In the case of bound constraints, the worst case cost of a single iteration ranges from $n + 1$ to $2n$ function evaluations, depending on the number of constraints, as is discussed in more detail in [32].

Subspace techniques in optimization

In the proposal "Managing the Choice of Surrogate Variables and the Use of Approximation Models to Optimize Expensive Functions," we suggested applying an optimization method to solve subproblems posed on subspaces of lower dimension and then applying the method (or possibly even a different optimization method) to solve the full-dimensional problem on the affine hull defined by the current iterate and the solutions found for the subproblems.

Subspace techniques would be useful in several ways. The biggest effect of dimension on the model management framework is that the construction of the approximations is based on sampling, using design of experiments to choose the interpolation sites that define the approximation. The number of points required quickly escalates with dimension—and the expensive objective has to be evaluated at each of these points. When we use interpolatory models as surrogates, we defer the curse of dimensionality that afflicts pattern search methods, but we do not eliminate it altogether, as we still must sample the search space to construct an initial approximation. Though it is less important, the problem of determining the data sites requires us to find as nearly as possible the global solution of an optimization problem. A different "global" optimization problem must be solved to determine the nonlinear interpolant which we will use as an approximation. Global optimization is nearly impossible even in low dimensions and global techniques becomes completely impractical in higher dimension. Furthermore, the model management framework, while less subject to dimensional effects than a standard pattern search technique applied directly to the expensive function, has some dimensional effect near a solution. However, it is doubtful that the subspace techniques will be of much help in that respect.

19

Fortunately, our original concerns about the efficacy of pattern search methods when used directly to solve problems with large numbers of variables did not prevent us from effectively tackling design problems with as many as 56 design variables—far larger than we had originally thought possible. In fact, pattern search methods have been successfully applied to optimization problems with as many as 256 variables. We still believe that even larger problems could be solved effectively using the subspace techniques and thus expect this subject to be a topic of future research.

Software

There are two distinct software products from this research: PDS and MMF. Of the two products, PDS is the more mature. It is also more widely applicable, easier to apply, and can be executed on either a sequential, parallel, or distributed computing platform. PDS is widely distributed and has been recognized as filling an important niche in the catalog of optimization software tools. On the other hand, MMF is a very new software product that currently exists as a Fortran 90 prototype. It has been transferred to Lawrence Berkeley Labs, to Sandia Labs, and to Boeing. We plan to transfer it to Mobil this year. The lack of high quality Fortran 90 compilers for various computing platforms has led Doug Moore to begin a C++ reimplementation, which will be completed by fall 1998. The C++ version will also be publicly available.

PDS

Torczon is in the process of completing a major revision of PDS, a software package for a family of parallel direct search methods for nonlinear optimization that can be executed on sequential, distributed, and parallel computing platforms. This family of optimization algorithms is described in Dennis and Torczon [21]; the ideas for these methods builds on the work found in Torczon [48, 49].

The original release of PDS was written using machine-specific libraries or compiler directives for implementations on a limited set of parallel computing platforms. With the help of David Serafini, the new release of the software now makes use of the Message Passing Interface (MPI) [44], which allows for generally seamless ports between all parallel and distributed computing platforms that support MPI. Once the external documentation has been completed and the implementation has passed through a final review, it will be resubmitted to *ACM Transactions on Mathematical Software* for publication.

PDS is also garnering increasing interest in the numerical software community. Serafini and Torczon were invited to install PDS on the Network-Enabled Optimization System (NEOS) Server at Argonne National Laboratory [18].[1] The invitation to install PDS on NEOS was extended both because PDS provides a family of robust techniques for handling optimization problems when derivatives are unavailable and finite-difference approximations are unreliable and because PDS is one of the few general-purpose, "scalable," parallel nonlinear optimization software packages.

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[1]URL: `http:/www.mcs.anl.gov/otc/Server/`

For the same reasons, Torczon has also been invited to submit PDS for inclusion in the Parallel Industrial Numerical Applications and Portable Libraries (PINEAPL), a project of the European Commission to develop parallel numerical library software for industrial applications.[2] This project is managed by the well-regarded Numerical Algorithms Group (NAG), Ltd., United Kingdom, an established software vendor with a large European industrial customer base (as well as a U.S. subsidiary and a U.S. customer base). In addition to including the parallel variant of PDS in PINEAPL, NAG has expressed an interest in incorporating the sequential variant into their commercial numerical libraries.[3] Final decisions will be made once the revision to the software has been completed and NAG has had a chance to exercise the extensive validation process that all software must pass to be included in the NAG numerical libraries.

Finally, Torczon has been asked to submit PDS for inclusion in the National HPCC Software Exchange (NHSE),[4] a program to actively promote software sharing and reuse within and across the twelve participating agencies[5] in the federal High Performance Computing and Communications (HPCC) Program. Development of the NHSE is being carried out by the Center for Research on Parallel Computation (CRPC).

MMF

The current version of the design document for MMF is available.[6] This file is changed as often as the design document is changed.

The heart of the framework is a C++ class called *Evaluable*, which encompasses all things that can be evaluated as functions, including Models, "Truth" and Memoizers that preserve function values to avoid expensive recalculation. Any Evaluable has a name, knowledge of its number of inputs and outputs, and the ability to have a subset of its outputs evaluated at a given input. It is intended that distinctions between objectives and various kinds of constraints be ignored at this level—higher-level "problem" objects know which components of the output vector are objectives, and which are constraints.

Memoizers offer the additional capability of reporting whether or not they have a stored output for a given input, and will offer proximity queries including functions to identify all the outputs for the inputs in a user-specified box, and to identify closest-matches to user-specified input points. The use of the well-supported Berkeley DB package, along with space-filling curve technology to minimize disk accesses, will make this an efficient solution to the archiving problem.

Models offer the additional capability of an "update" method, in which an input/output pair from "truth," or from a more accurate model, is used to improve the current model.

Other important classes in the implementation are *ModeledOptProblems*, which know which parts of an evaluable output are objectives and which are constraints; *TrialSolutions*, which record an input, the corresponding output, and a radius in which a better answer is

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[2]URL: `http://extweb.nag.co.uk/projects/PINEAPL.html`

[3]URL: `http://www.nag.co.uk.numeric.html`

[4]URL: `http://www.nhse.org`

[5]NIST, AHCPR, DARPA, NOAA, NASA, EPA, VA, NIH, NSF, ED, NSA, and DOE.

[6]URL: `http://www.caam.rice.edu/ dougm/MMF2.design.ps`

likely to lie; *Terminators*, which decide when to abandon a search; *Searches*, which recommend points that might improve the objective; *Polls*, which describe optimization fallback strategies; and various utility classes.

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